Correlation Coefficients in Lee´s Model of Multiphase Flows

Natália Holešová[1,*], *Richard* Lenhard[1], *Katarína* Kaduchová[1] and *Milan* Malcho[1]

[1]Department of Power Engineering, Faculty of Mechanical Engineering, University of Žilina, Univerzitná 1, 010 26 Žilina, Slovakia

Abstract. Multiple technical and biological systems exhibit multiphase flow phenomena. The demands for accurate calculations of the physical phenomena that occur in engineering technologies have increased along with their rapid advancement. However, it is very hard to identify two- and multi-phase flow through experimental measurements, as a result, in addition to experimental measurements, numerical simulations are also performed, which can help improve our physical understanding of the complex phenomenon of phase transformations. The goal of numerical simulations of phase changes is to precisely simulate the real progress and experiment. These simulations operate on the basis of physical principles and correlation coefficients of phase changes. These correlation coefficients have a different range of values. The examination of the Lee model's correlation coefficients from the ANSYS Fluent environment, which is now the most popular for multiphase flow simulations, is the subject of the article that is being given. In this article is also described and tested the numerical simulation of interphase mass transport in a closed space.

Research background: The article is focused on the problematics of multiphase flows. In ANSYS Fluent, there are many types of models, which are used for the numerical simulations of this phenomena. In models are included correlation parameters, which are specific for every single situation and are within the given ranges. This paper is about the Lee model, which correlation coefficients are in the range from 10^{-3} to 10^{2}.
Purpose of the article: A detailed description of Lee's model with its testing on a heat pipe in the ANSYS Fluent program with determined correlation coefficients.
Methods: The use of CFD simulation of multiphase flow to determine correlation coefficients.
Findings & Value added: Testing the correlation coefficients of Lee's model and finding their appropriate values for the given situation.

Keywords: *Lee model, correlation coefficient, CFD simulation, multiphase flow*

* Corresponding author: natalia.holesova@fstroj.uniza.sk

1 Introduction

A unique characteristic of two-phase or two immiscible mixtures is the presence of one or more interfaces separating the phases or components. Examples of such flow systems can be found in a large number of engineering systems as well as in a wide variety of natural phenomena. Understanding the flow and heat transfer processes in two-phase systems is becoming increasingly important in nuclear, mechanical, and chemical engineering, as well as in the environmental and medical fields.

The design of engineering systems and the ability to predict their performance depend on the availability of experimental data and conceptual mathematical models that can be used to describe physical processes with the required degree of accuracy. It is imperative that the various characteristics and physics of two-phase flow be modelled and formulated on a rational basis and supported by detailed scientific experiments.

The evaporation and condensation are also included, which are crucial components of many important industrial processes, among the two-phase flow.

Evaporation is the process of turning a liquid into vapor at its saturation temperature, by the action of heat. Condensation, which is the reverse of evaporation, occurs when heat is removed from or absorbed by a vapor, turning it into a liquid. To understand the evaporation and condensation phenomena, several experimental analyses have been conducted. However, it is very difficult to detect these phenomena with experimental measurements, and therefore numerical simulations are usually performed with experimental measurements.

Numerical simulations can contribute to a better physical understanding of the complex phenomena of phase transformations - evaporation and condensation. The ANSYS Fluent program is currently the most widely used CFD analysis software, which enables multiphase flow modelling with heat and mass sharing for liquid-gas, liquid-solid phase combinations, and fluid-solid interaction.

The aim of the article is to describe the correlation coefficient of the Lee model, which is used for numerical simulations of interphase heat transport in a closed space, taking into account condensation and evaporation. This coefficient must be correlate to match the experimental data as closely as possible.

1.1 Lee model

Nowadays, there are already many different types of phase change models [10]. Using empirical expressions to quantify interfacial heat and mass transfer appears to be a common way to model phase change phenomena. This approach is indeed useful for certain simple geometries but limited for any other more complex geometry.

The phase change model proposed by Lee is the most commonly used. Mass transfers are given by the following equations [6], [8], [11], [13]:

If $T_l > T_{sat}$ (evaporation)

$$\dot{m}_{lv} = \lambda_c \alpha_l \rho_l \frac{T_l - T_{sat}}{T_{sat}} \tag{1}$$

If $T_v < T_{sat}$ (condensation)

$$\dot{m}_{vl} = \lambda_c \alpha_v \rho_v \frac{T_{sat} - T_v}{T_{sat}} \tag{2}$$

where $\dot{m}_{lv}, \dot{m}_{vl}$ are intensities of mass transfer due to evaporation and condensation, respectively (kg.s^{-1}.m^{-3}); α_l, α_v are phase volumes fractions (–); ρ_l, ρ_v are densities of liquid and vapor (kg.m^{-3}); T_l is the temperature of liquid (K); T_{sat} is the temperature of saturation (K) and T_v is temperature of vapor (K). λ_c denotes the mass transfer intensity factor with unit s^{-1}. It is recommended that the value of λ_c be such that it keeps the interfacial temperature reasonably close to the saturation temperature and avoids divergence problems [14].

As an empirical coefficient, λ_c has different values for different situations [9]. In numerical studies by Wu et al. [1], De Schepper et al. [2] and Alizadehdakhel et al. [3], λ_c was set to 0.1 s^{-1} and 1 s^{-1} to numerically keep the interface temperature close to the saturation temperature. However, in Yang [4] and Fang [5], λ_c was specified at a different value, 100 s^{-1}.

λ_c, which is inverse to relaxing time (s^{-1}) is defined:

$$\lambda_c = \frac{6}{d_b}\,\beta\sqrt{\frac{M}{2\pi R T_{sat}}}\,L\left(\frac{\alpha_v \rho_v}{\rho_l - \rho_v}\right) \tag{3}$$

where d_b is diameter of bubble (m); β is adaptation coefficient, which shows a part of the vapor molecules moving to the surface of the liquid and subsequently being absorbed by this surface (-); M is molar mass (kg.mol^{-1}); T_{sat} is saturation temperature (K); R is universal gas constant (J.K^{-1}.mol^{-1}); L is latent heat (J.kg^{-1}); α_v is phase volume fraction (-); ρ_v, ρ_l are densities of vapor and liquid (kg.m^{-3}).

This leads to the final expression for the evaporation process defined by equation (1). It can be considered implicitly as the source term in the conservation phase of the equation. A similar term can be obtained by condensation. In this case, even small droplets in the continuous gas phase regime are considered, even if the primary phase is liquid.

The coefficient λ_c should theoretically be different for condensation and evaporation. In addition, the theoretical expression is based on several assumptions:

- desktop interface,
- diffuse mode with constant diameter,
- known β.

The bubble diameter and the fitting coefficient are usually not known, which is why the coefficient λ_c must be tuned to match the experimental data. By default, the coefficient for evaporation and condensation is 0.1 s^{-1}. However, λ_c in practical cases can reach a value of the order of 10^2 s^{-1}.

2 Numerical simulation of multiphase flow in an enclosed space

The 2D model of the numerical non-stationary simulation of interphase mass transport in a closed space in the ANSYS Fluent program is a gravity heat pipe, which consists of an evaporative, adiabatic, and condensing part. The heat pipe contains water, steam, and a non-condensing component - air. The detail of the 2D model and the main dimensions are described in Figure 1 and Table 1.

Table 1. Dimensions of heat pipe.

V11	400 mm	V15	120 mm
V12	80 mm	V16	52 mm
H8	32 mm		

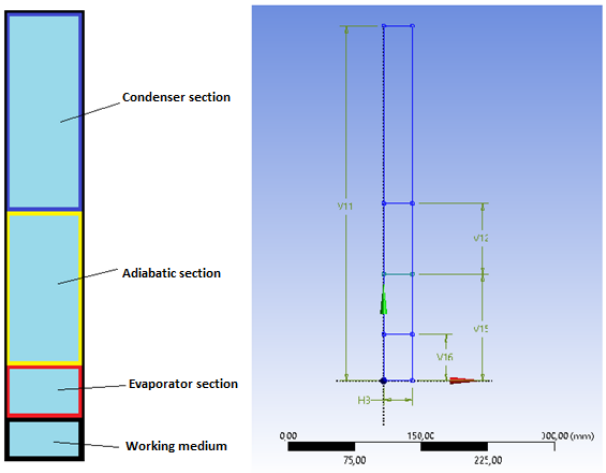

Fig. 1. Geometric parameters of heat pipe.

In multiphase mass transport (condensation and evaporation), it is important to pay attention to the modelled phenomena and adapt the computational mesh to capture these types of heat transport. During condensation and evaporation, it is necessary to thicken the mesh near the walls and just above the surfaces of the working substances, where phase changes occur. A square mesh with 57 256 cells was used to create the 2D model of the heat pipe. The Evaporation – Condensation model was used to describe the multiphase heat transport of mass, the settings of which are contained in the following tables with a description of the parameters of boundary, operational, material, and other key conditions. Data are obtained from experimental measurement and used as input values for numerical simulation. The values of the correlation coefficients are set to 0.1 s^{-1} and 10 s^{-1}, which describe the best our experiment.

Table 2. Boundary conditions.

Name	**Type of condition**	**Set parameters**		
		Velocity [m.s^{-1}]	**Temperature [°C]**	**Temperature flow [W.m^{-2}]**
chladenesteny	Wall	0	10	–
adiabatickacast	Wall	0	–	0
ohrievanesteny	Wall	0	200	–

Table 3. Operational conditions.

Pressure [Pa]	**Boiling temperature [°C]**	**Gravitation [m.s^{-2}]**
20 000	60	- 9,81

Table 4. Material conditions.

Material	Density [kg.m^{3}]	Thermal capacity [J.kg^{-1}.K^{-1}]	Thermal conductivity [W.m^{-1}.K^{-1}]	Dynamic viscosity [kg. m^{-1}.s^{-1}]
Air	1.225	1 006.43	0.0224	1.7894×10^{-5}
Water	998.2	4182	0.6	1003
Mixture	0.13	*	0.0261	1.34×10^{-5}

*cp (T) = $1563.077 + 1.603755T - 0.002332784T^2 + 3.216101\times10^{-6}T^3 - 1.156527\times10^{-9}T^4$

Table 5. Material conditions.

Material	Molar mass [kg. kmol^{-1}]	Enthalpy [J. kmol^{-1}]	Reference temperature [°C]
Air	28.966	0	25
Water	18.0152	0	25
Mixture	18.01534	4.399×10^{7}	25

Table 6. General conditions.

Space dimension	Precision	Flow	Setting of the model
2D	double	Non-stationary	evaporation - condensation: T_{var} = 60 °C, λ_l **= 0.1,** λ_v **= 10**
		Non-compressible, laminar	Multiphase model: mixture Liquid phase = water, Gaseous phase (mixture) = water vapor + air

Table 7. Setting of the solution.

Type	Coupling	Discretization	Discretization of pressure	Transient formulation
Pressure-based	Simple	1st order upwind	Standard	1st order implicit

Table 8. Under-relaxation factors.

Under-relaxation factors	
Density	0.9
Body Forces	0.9
Pressure	0.3
Momentum	0.7
Species	0.9
Energy	0.7
Volume Fraction	0.5
Slip Velocity	0.1
Vaporization Mass	0.9

Table 9. Setting of the solution.

Time stepping method	Time step size	Number of time steps	Max iterations	Reporting interval
Fixed	0.001	10 000	20	1

3 Results of numerical simulation

Even before starting the numerical calculation, it was necessary to correctly patch the phases where water and air are located. In Figure 2 individual phases are plotted through the Volume Fraction contour.

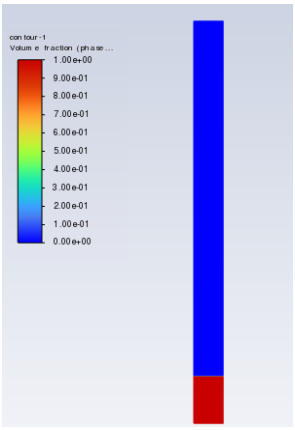

Fig. 2. Initial state of Volume Fraction from stationary simulation; phase-1 is water.

The simulation was set to calculate 10 000 numbers of time steps with 0.001 time step size, which means that the simulation captures 10 s of heat pipe heating. In Figure 3, it is possible to see the formation of a steam bubble at water in 2 s.

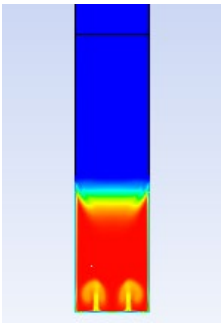

Fig. 3. The presence of steam bubble in the bottom of heat pipe.

Other figures show the time courses of state changes in a heat pipe. Figure 4 shows the time course of the density at times 0.5 s, 1 s, 2 s, 5 s and 10 s. At the same times, speed (Figure 5.) and temperature (Figure 6.) are also shown.

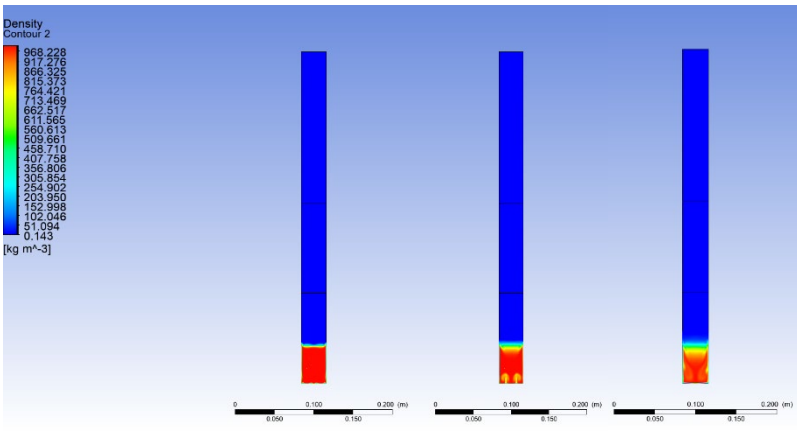

Fig. 4. Contours of densities at times 0.5 s, 1 s, 2 s.

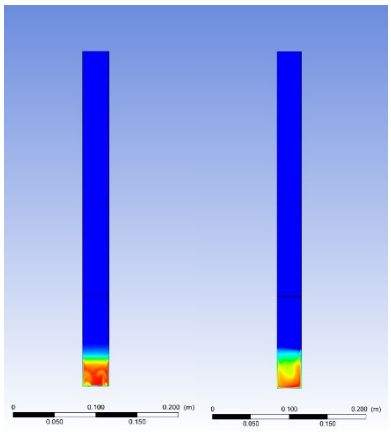

Fig. 5. Contour of density in 5 s and 10 s.

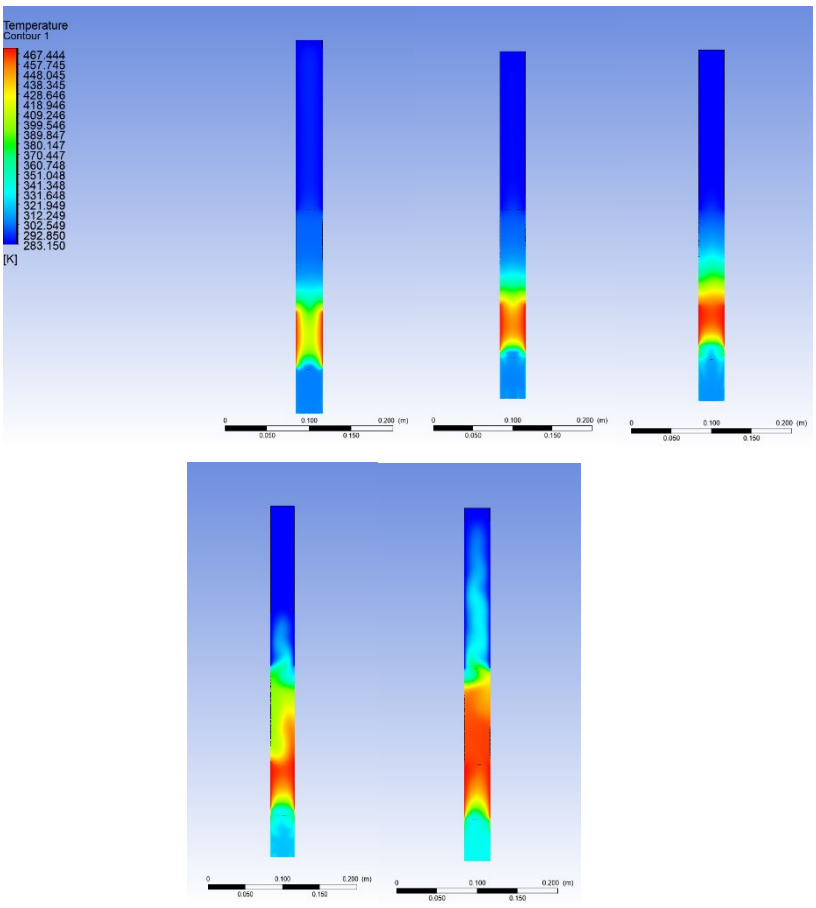

Fig. 6. Contours of temperatures at the times 0.5 s, 1 s, 2 s, 5 s, 10 s.

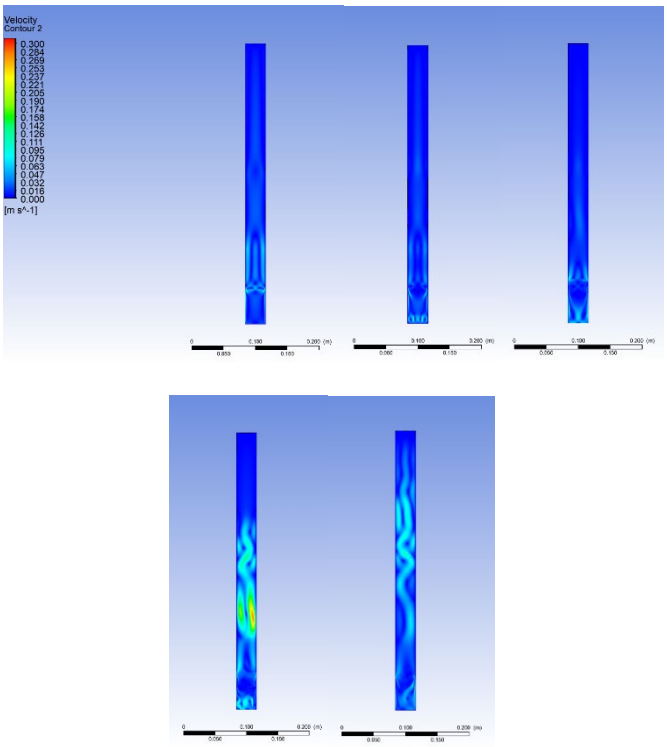

Fig. 7. Countours of velocities at the time 0.5s, 1s, 2s, 5s, 10s

4 Conclusion

In general, this article analyses the mathematical model of multiphase flow - the Lee model, which uses the ANSYS Fluent program for numerical simulations of heat transfer in multiphase flows. Lee's model includes certain correlation coefficients in its mass transfer relations. These correlation coefficients must be fine-tuned that they describe the real experimental measurement as accurately as possible. They depend on the amount of condensate formed and reach values from 10^{-3} to 10^{2} s^{-1}.

The output of the article is numerical simulation of interphase mass transport in a closed space - heat pipe capturing physical phenomena – evaporation with an optimized correlation coefficient of the Lee model - λ_c were 0.1s^{-1} and 10 s^{-1}. These coefficients are valid only for the given situation when pressure is 20 000 Pa and boiling temperature is 333.15 K.

In the future, by carrying out the experiment to obtain experimental data on the generated condensate and subsequent back-calculation of the correlation coefficients in program ANSYS Fluent, the dependence of the correlation coefficient on the amount of generated condensate would be created, thanks to which it would be able to create a correlation graph that would be used to refine the CFD simulation to a real experimental measurement.

This research is supported by the project KEGA 047ŽU-4/2022 Innovative approaches to fluid dynamics modelling in energy systems and KEGA 046ŽU-4/2021 Innovative methods of increasing the thermal efficiency of small heat sources using heat recovery through phase transformations.

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